Density-matrix functionals with local interactions

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Dynamical-Mean-Field-Theory (DMFT) calculations have shown that local interactions, i.e. the Anderson impurity model, capture a range of interesting correlation effects. We present first developments towards a method that incorporates such correlation effects into the standard methodology of DFT-based ground-state first-principles calculations. The method is based on density matrix functional theory with a functional obtained on the fly with a full CI ansatz. The validity of the methodology has been explored using simple model Hamiltonians. As a first step towards a full implementation into the CP-PAW code, the density-matrix functional has been approximated by a hybrid functional, namely PBE0. This corresponds to a PBE0 calculation with completely screened intersite interaction, i.e. PBE0(r). Not only a d- or f-shell, but all orbitals including core states from a given site participate in the explicit Fock term. Compared to a complete implementation of hybrid functionals, the computational overhead of this method is negligible. Results for transition metal oxides are presented.